The Eurasia Proceedings of Science, Technology,
Engineering & Mathematics (EPSTEM)
ISSN: 2602-3199

The Eurasia Proceedings of Science, Technology, Engineering & Mathematics (EPSTEM), 2019

Volume 7, Pages 363-370

IConTES 2019: International Conference on Technology, Engineering and Science

Evaluation of Theoretical and Experimental Spectroscopic Properties of 3-Methyl-4-[4-methoxy-3-(*p*-toluenesulfonyloxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one

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Abstract: In this study, 3-methyl-4-[4-methoxy-3-(p-toluenesulfonyloxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one was synthesized according to literature. Experimental data were obtained from the literature. The synthesized title compound was optimized by using B3LYP/6-311G(d,p) basis set. ^{1}H-NMR and ^{13}C-NMR spectral data values were calculated according to the method of gauge including atomic orbital (GIAO) and continuous set of gauge transformations (CSGT) methods using the program package Gaussian G09W Software. Experimental and theoretical values were inserted into the graphic according to equitation of δexp=a+b. δ calc. The standard error values were found via SigmaPlot program with regression coefficient of a and b constants. Also, the calculated IR data of compound were calculated in gas phase by using of 6-311G(d,p) basis set of B3LYP method and are multiplied with appropriate adjustment factors. Theoretical infrared spectrums are formed from the data obtained according to B3LYP method. In the identification of calculated IR data was used the veda4f program. The calculated and experimental results were exhibited a very good agreement.

Keywords: 1,2,4-Triazol-5-one, GIAO, CSGT, B3LYP, Experimental, Theoretical

Introduction

Heterocyclic compounds that possess 1,2,4-triazole ring have relevance to the pharmacological properties. These properties are fungicidal, antioxidant, antimicrobial, anticancer and antiviral activities (Li et al., 2004; Kritsanida et al., 2002; Holla et al., 2002; Gürsoy Kol and Yüksek, 2010; Sancak et al., 2010; Çiftçi et al., 2018). In addition to this kind of relevance, it was reported that Schiff bases that were originated from triazole compounds possessed some biological activities (Çiftçi et al., 2018). Triazole derivatives have been widely used as antifungal agents, especially, many known triazole agents presently play a leading role in the treatment of agricultural fungal infections, including epoxiconazole, tebuconazole and triadimefon, et al. What's more, triazole agents have a big market share in the field of pesticide because of strong systematic and unique mechanism property.

Density functional theory calculations (DFT) are reported to showed excellent vibrational frequencies of organic compounds if the calculated frequencies are scaled to compensate for the approximate treatment of electron correlation, for basis set deficiencies and for the anharmonicity (Abramov et al., 1999; Handy et al., 1992). A number of papers have recently appeared in the literature concerning the calculation of Nuclear Magnetic Rezonans chemical shift by quantum-chemistry methods (Forsyth and Sebag, 1997; Sebag et al., 2001; Turhan Irak and Gümüş, 2017; Beytur et al., 2019; Turhan Irak and Beytur, 2019). These papers indicate that geometry optimization is a crucial factor in an accurate determination of computed NMR chemical shift. Moreover, it is known that the DFT (B3LYP) method adequately takes into account electron correlation contributions, which are especially important in systems containing extensive electron conjugation and/or electron lone pairs (Forsyth and Sebag, 1997). However, considering that as molecular size increases, computing-time limitations are introduced for obtaining optimized geometries at the DFT level, it was proposed that the single-point calculation

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of magnetic shielding by DFT methods was combined with a fast and reliable geometry-optimization procedure at the molecular mechanics level (Forsyth and Sebag, 1997).

The gauge-including atomic orbital (GIAO) (Ditchfield, 1972, Wolinski et al., 1990) method is one of the most common approaches for calculating nuclear magnetic shielding tensors. It has been shown that the results obtained by GIAO method are often more accurate than those calculated with other approaches, at the same basis set size (Cheeseman et al., 1996). DFT methods have been preferred in the study of large organic molecules (Friesner et al., 1999) and for GIAO ^{13}C calculations (Cheeseman et al., 1996) in all those cases in which the electron correlation contributions were not negligible.

Density Functional Theory (B3LYP) methods are used for the determination of the structure of molecules and the investigated of spectroscopic properties. Firstly, 3-methyl-4-[4-methoxy-3-(p-toluenesulfonyloxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one compound was obtained according to the literature (Aktaş Yokuş, 2012). The compound was analyzed with IR, ^{1}H-NMR and ^{13}C-NMR and experimental spectrums were drawn. The titled compound has been optimized using B3LYP/6311G(d) basis set (Frisch et al., 2009; Wolinski et al., 1990). ^{1}H-NMR and ^{13}C-NMR isotropic shift values were calculated by the methods of GIAO and CSGT using the program package Gaussian G09W (Frisch et al., 2009). Experimental (Aktaş Yokuş, 2012) and theoretical values were inserted into the graphic according to equitation of $\delta\ \mathrm{exp}_{=}a+b.\ \delta$ calc. The standard error values were found via SigmaPlot program with regression coefficient of a and b constants. IR absorption frequencies of analyzed molecule were calculated by two methods. The veda4f program was used in defining IR data, which were calculated theoretically (Jamróz, 2004).

Computational Details

The title compound was optimized based on the 3-methyl-4-[4-methoxy-3-(p-toluenesulfonyloxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one. The optimized molecular structures of the title compound in the ground state (in vacuo) were computed by performing DFT by a hydrid functional B3LYP functional (Becke's three parameter hybrid functional using the LYP correlation functional) methods (Becke, 1993; Lee, 1998) at 6-311G(d,p) level. The gauge-including atomic orbital (GIAO) (Ditchfield, 1974; Rohling et al., 1984; Wolinski et al., 1990) and continuous set of gauge transformations (CSGTs) (Keith and Bader, 1992) methods are three of the most common approaches for calculating nuclear magnetic shielding tensors (Pir et al., 2013, Rani et al., 2010; Turhan Irak and Beytur, 2019; Beytur et al., 2019). In the present study, ^{1}H and ^{13}C NMR chemical shifts were calculated within GIAO and CSGT approach applying B3LYP method with 6-311G(d,p) basis set.

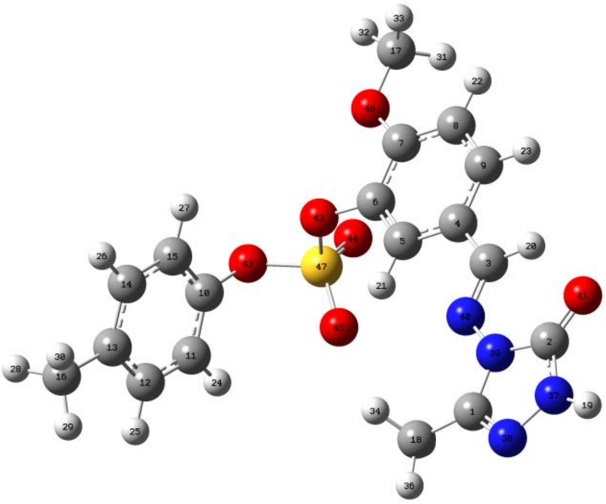

Figure 1. The optimized molecular structure of 3-methyl-4-[4-methoxy-3-(p-toluenesulfonyloxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one with DFT 6-311G(d,p) level.

Results and Discussion

NMR spectra of 3-methyl-4-[4-methoxy-3-(p-toluenesulfonyloxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one

In nuclear magnetic resonance (NMR) spectroscopy, the isotropic chemical shift analysis allows us to identify relative ionic species and to calculate reliable magnetic properties which provide the accurate predictions of molecular geometries (Rani et al., 2010; Subramanian, Sundaraganesan, & Jayabharathi, 2010; Wade, 2006). Initially, molecular structure of 3-methyl-4-[4-methoxy-3-(p-toluenesulfonyloxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one is optimized by using B3LYP method with 6-311G(d,p). Then, both GIAO and CSGT ^{13}C and ^{1}H calculations of the title compound have been made by using B3LYP method with 6-311G(d,p) basis set. The GIAO and CSGT methods according to ^{1}H and ^{13}C chemical shift values (with respect to TMS) have been calculated for the optimized structures of the title compound and compared to the experimental 1H chemical shift values (Aktaş Yokuş, 2012) (Table 1). In the present paper, ^{1}H-NMR and ^{13}C-NMR spectral data values were calculated according to the method of gauge including atomic orbital (GIAO) and continuous set of gauge transformations (CSGT) methods using the program package Gaussian G09W Software. Theoretical and experimental (Aktaş Yokuş, 2012) values were plotted according to δ exp=a. δ calc.+ b, Eq. a and b constants regression coefficients with a standard error values were found using the SigmaPlot program.

Table 1. Data calculated ^{13}C and ^{1}H-NMR DMSO(B3LYP/6311G(d,p) isotropic chemical shifts of the molecule according to GIAO and CSGT Methods (δ/ppm)

No	Experim.	DFT/6311(d,p) DMSO GIAO	Diff./DMSO	DFT/6311(d,p) DMSO CSGT	Diff/DMSO
1C	146,18	150,35	-4,17	147,56	-1,38
2C	152,63	153,59	-0,96	147,95	4,68
3C	151,65	152,10	-0,45	151,68	-0,03
4C	126,73	131,02	-4,29	130,17	-3,44
5C	121,35	123,63	-2,28	121,22	0,13
6C	132,51	144,02	-11,51	141,74	-9,23
7C	154,33	161,77	-7,44	158,88	-4,55
8C	114,02	114,59	-0,57	114,11	-0,09
9C	129,87	137,93	-8,06	137,62	-7,75
10C	144,59	154,11	-9,52	152,29	-7,70
11C	128,75	127,87	0,88	126,05	2,70
12C	130,38	134,14	-3,76	133,24	-2,86
13C	138,50	146,39	-7,89	145,72	-7,22
14C	130,38	134,26	-3,88	133,48	-3,10
15C	128,75	127,17	1,58	125,57	3,18
16C	21,61	21,31	0,30	23,40	-1,79
17C	56,45	55,76	0,69	46,43	10,02
18C	11,44	12,43	-0,99	13,51	-2,07
19H	11,80	7,25	4,55	7,20	4,60
20H	9,86	10,01	-0,15	9,12	0,74
21H	7,89	7,93	-0,04	7,65	0,24
22H	7,28	7,00	0,28	7,15	0,13
23H	7,62	7,52	0,10	7,41	0,21
24H	7,72	7,38	0,34	7,38	0,34
25H	7,47	7,50	-0,03	7,66	-0,19
26H	7,47	7,51	-0,04	7,68	-0,21
27H	7,72	7,56	0,16	7,55	0,17
28H	2,43	2,57	-0,14	3,11	-0,68
29H	2,43	2,23	0,20	2,71	-0,28
30H	2,43	2,35	0,08	2,84	-0,41
31H	3,62	3,76	-0,14	4,24	-0,62
32H	3,62	4,3	-0,68	4,82	-1,20
33H	3,62	3,88	-0,26	4,32	-0,70
34H	2,09	2,17	-0,08	2,56	-0,47
35H	2,09	2,22	-0,13	2,6	-0,51
36H	2,09	1,93	0,16	2,29	-0,20

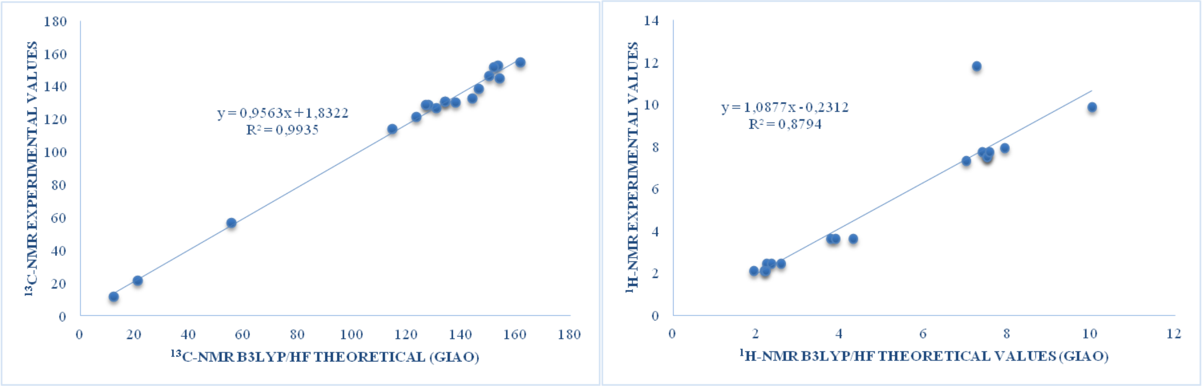

Figure 2. The correlation graphics for ^{13}C-NMR (DMSO) and ^{1}H-NMR (DMSO) chemical shifts of the molecule according to GIAO

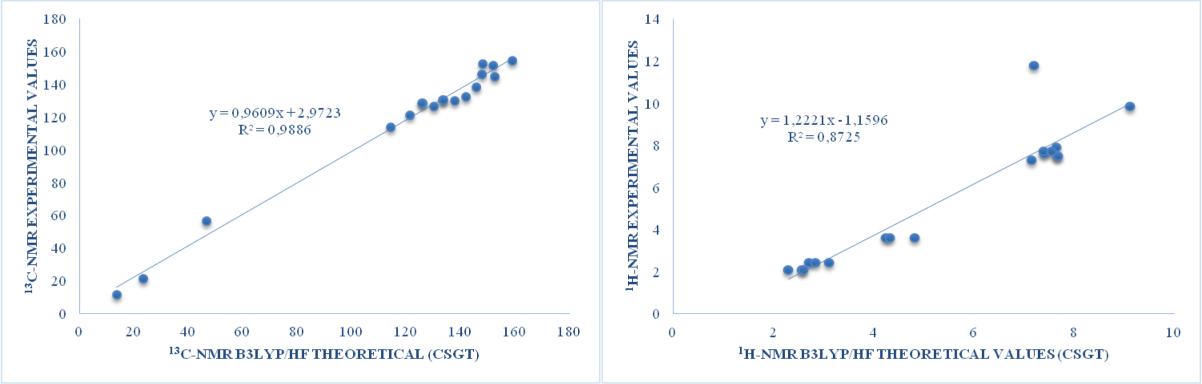

Figure 3. The correlation graphics for ^{13}C-NMR (DMSO) and ^{1}H-NMR (DMSO) chemical shifts of the molecule according to CSGT

The relation between R^2 values of the compound

B3LYP/6311G(d,p) (GIAO): ^{13}C: 0.9935, ^{1}H: 0.8794 and B3LYP/6311G(d,p) (GIAO): ^{13}C: 0.9886, ^{1}H: 0.8725. There is such a relationship between R^2 values of the 3-methyl-4-[4-methoxy-3-(p-toluenesulfonyloxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one. Found standard error rate and a, b constants regression values were calculated according to formula exp =a +b.δ calc Eq.

Assignments of the vibrational modes of the compound

Experimental vibrational data of the title compound has been taken by from (Aktaş Yokuş, 2012). We have calculated the theoretical vibrational spectra of the title compound using B3LYP method with 6-311G(d,p) basis set. We have compared our calculations of the title compound with the experimental results and the comparison is shown in Table 2. The vibrational bands assignments have been made by using Gauss-View Molecular Visualisation Program (Frisch et al., 2003). To make comparison with experiment, we present correlation graphic in Figure 3 based on the calculations. As we can see from the graph in Figure 3 experimental data are in better agreement with the scaled data and are found to have a good correlation for B3LYP. Theoretically IR values were calculated with the veda4f program and scalar values were obtained. The negative frequency in the data was not found. This result shows that the structure of compound was shown to be stable. IR spectrums were drawn with obtained values according to DFT method. Theoretical IR values were compared with experimental IR counterparts. The result of this compare were found corresponding with each other of values (Aktaş Yokuş, 2012).

As can be seen from Table 2, the N-H vibrations of the title compounds have been calculated by using B3LYP method with 6-311G(d,p) basis set observed at 3148 cm^{-1} (Aktaş Yokuş, 2012). This vibration band was calculated at 3647 cm^{-1} (for B3LYP). The C=O experimental vibrations band of title compound were observed at 1689 cm^{-1}, that have been calculated with B3LYP at 1787 cm^{-1} (see Table 2). As can be seen from Table 2, there is good agreement beetween experimental and theoretical vibration data for the C–H asymmetric and symmetric stretch and the others.

Table 2. The calculated frequencies values of the molecule.

Vibration Types	Experimen.	B3LYP
COSO (83)		5
CCOS (19), OSOC (49)		14
OSOC (23), NCCC (28), CNNC (15)		19
OSOC (24), HCCC (43)		27
HCCC (10), CCOS (31), OSOC (18)		29
OSOC (38), HCCC (22)		32
CCCC (14), NCNN (14), NNCN (11), COCC (11)		44
NCC (24), CCC (20), CCOS (13)		61
COS (25), CCCO (13), OSOC (11)		80
NCNN (13), CNNC (21), COCC (17)		91
CNNC (30)		157
NCCC (24), CNNC (20)		189
OSO (24), CCCO (10)		223
CNNC (47), HNNC (19)		295
CCO (12), CCN (12), COC (10), OOOS (15)		308
CCCO (45), CCCC (10), NNCN (10), NCNN (16)		317
CNN (18), OCN (15), NNC (10), CCN (14)		359
OCCC (16), CCCC (11)	406	416
OCC (20), OSO (18)		434
HNNC (51), ONNC (11)		457
OSO (31)		481
OSO (12), CCCO (10), CCCC (14), OCCC (13)	479	498
OOOS (44)		525
CCO (18)	542	556
OOOS (10)	581	579
CC (11), OCN (12), CNN (12)		604
CC (18)	626	629
CCCC (10)		638
CCC (46), OCC (10)	665	648
ONNC (76)	721	738
CC (15), CCC (24)	761	782
CC (14), SO (15), CCC (11)		794
NC (20), CNN (36)		800
HCCC (72), OCCC (11)	813	819
HCCC (59), CCCC (10)		859
CCCC (10), HCCC (59)	900	909
HCCC (81)	951	966
HCH (12), NNC (10), HCCN (33)		987
HCH (18), HCCC (54)		999
CCC (66)		1026
CCC (11), OC (67)	1014	1043
HCH (19), HCCC (54)		1053
HCH (21), HCCN (69)		1058
NN (38), HNN (10), HCCN (17)	1087	1093
CC (22), HCC (39)		1120
OC (13), SO (46)		1143
HCH (13), HCOC (65)		1160
HCOC (38)	1179	1197
NC (12), HCOC (129)		1202
CC (54)		1219
CC (14), HCC (23)		1231
HCC (29)		1266
NCN (12)	1277	1292
NN (13), NCN (129)		1296

NC (24), HCN (26), HCH (18)	1309	**1314**
NC (24), HCN (26), HCH (10)	1361	**1368**
HCH (16), HNN (58)		**1383**
NC (10), HCN (16), HCH (14)		**1440**
CC (41), HCC (13)	1429	**1443**
HCH (76), HCCN (22)		**1458**
HCH (77)		**1465**
HCH (75), HCCC (16)	1457	**1477**
HCOC (23), HCH (75)		**1481**
HCH (67), HCCC (14)		**1483**
OC (14), CCC (14), HCC (25)	1510	**1531**
CC (51), CCC (10)		**1586**
CC (21), NC (20)		**1628**
NC (60)	1599	**1650**
NC (13), OC (73)	1689	**1787**
CH (99)	2643	**2984**
CH (91)		**3017**
CH (98)	3049	**3071**
CH (91)		**3113**
CH (98)		**3117**
CH (98)		**3122**
CH (100)		**3137**
CH (97)		**3140**
CH (98)		**3143**
CH (94)		**3177**
CH (93)		**3178**
CH (99)		**3182**
CH (98)	3148	**3189**
NH (100)	3252	**3647**

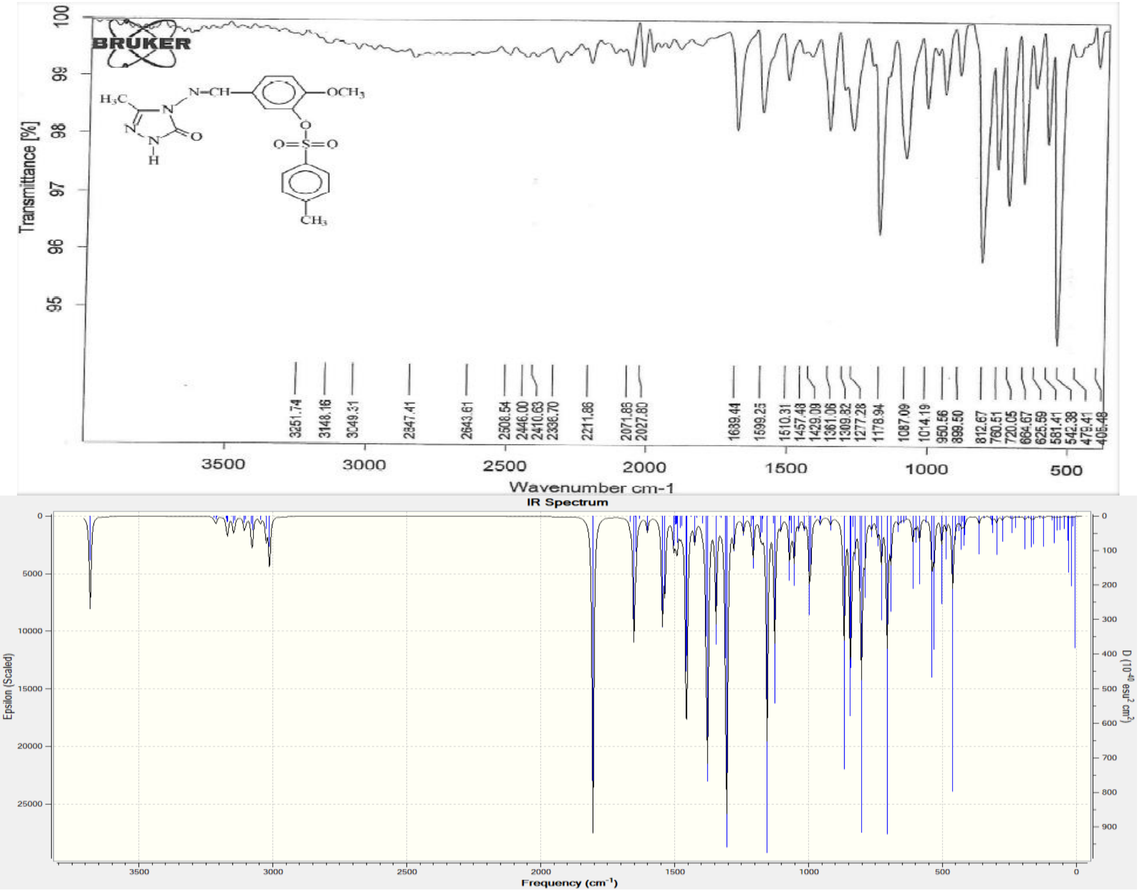

Figure 3. IR spectra experimental and simulated with DFT/B3LYP/6311G(d,p) levels of the molecule

Conclusion

In this work we have calculated the vibrational frequencies and ^{13}C NMR and ^{1}H NMR chemical shift values of the title compound (3-methyl-4-[4-methoxy-3-(p-toluenesulfonyloxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one) by using B3LYP method with 6-311G(d,p) basis set. To fit the theoretical vibrational frequency results with experimental ones for B3LYP we have multiplied the data by 0.9905. Multiplication factors results gained seemed to be in a good agreement with experimental data. In particular, the results of B3LYP method has shown better fit to experimental data in evaluating vibrational frequencies. Likewise, B3LYP method seems to be appropriate for the calculation of geometrical parameters of molecules.

To test the different theoretical approaches (DFT/B3LYP) reported here, computed and vibrational frequencies and ^{1}H NMR and ^{13}C NMR chemical shift values according to GIAO and CSGT methods of the 3-methyl-4-[4-methoxy-3-(p-toluenesulfonyloxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one were compared. More commonly, however, the IR and NMR spectra are used in conjunction with other forms of spectroscopy and chemical analysis to determinate the structures of complicated organic molecules.

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